

Wigner crystal *vs.* Friedel oscillations in the 1D Hubbard model

Stefan A. Söffing, Michael Bortz, Imke Schneider, Alexander Struck, Michael Fleischhauer, and Sebastian Eggert

*Dept. of Physics and Research Center OPTIMAS,
Univ. Kaiserslautern, D-67663 Kaiserslautern, Germany*

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We analyze the fermion density of the Hubbard model in a finite one-dimensional system. A Wigner crystal phase should not be expected, since there cannot be any broken symmetry in one dimension and moreover the underlying Luttinger liquid theory is scale invariant. Nonetheless, we find a relatively sharp crossover even for moderate short range interactions into a definite Wigner crystal region. The results are relevant to ultra cold fermionic gases in optical lattices and finite quantum wires.

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Having been predicted in the early days of quantum mechanics, the Wigner crystal[1] is one of the simplest but most dramatic many-body effects: Due to the long range repulsive forces, electrons spontaneously form a self-organized lattice at low enough densities and temperatures much different from a free electron gas. Experimental verification has been difficult, but very recently experimental signatures of a Wigner crystal were reported in carbon nanotubes[2]. Using ultra cold gases in optical lattices it is now also possible to produce well-controlled correlated fermion systems in restricted dimensions, albeit with *short range* interactions[3, 4].

The Wigner crystal in one dimension has been discussed so far mostly in the context of long-range interactions. In that case it has been predicted by Schulz [6] that the density-density correlations corresponding to an equally spaced inter-particle distance become dominant. Numerically a crossover to Wigner density waves has been observed at strong long-range interactions with very few particles[7]. However, for *short-range* interacting fermion systems in one dimension possible Wigner crystal signatures have not been addressed theoretically so far.

The prototypical model for short range interacting fermions is the repulsive ($U > 0$) one-dimensional (1D) Hubbard model

$$H = -t \sum_{x=1}^{L-1} \left(\psi_{\sigma,x}^\dagger \psi_{\sigma,x+1} + h.c. \right) + U \sum_{x=1}^L n_{\uparrow,x} n_{\downarrow,x}. \quad (1)$$

Even though many exact results have been derived for this model using the Bethe Ansatz[5], the local densities in finite chains with open boundaries cannot yet be calculated by exact methods.

Since the on-site scattering is independent of momentum, the system becomes effectively scale invariant at low energies, so that any crossover towards a different physical region would be unexpected. Moreover, a Wigner crystal region should be unstable, since $2k_F$ -density Friedel oscillations [8] are always the slowest decaying correlations due to a limited Luttinger parameter[6] $0.5 \leq K_c \leq 1$. Nonetheless, sub-dominant

oscillations at other wave-vectors also exist as has been explicitly shown e.g. for the Hubbard model in a finite magnetic field[9, 10].

We now study the density distribution in finite Hubbard chains with hard-wall boundaries by a combination of bosonization and numerical density matrix renormalization group (DMRG) calculations. Despite the fact that the interactions are short ranged and of moderate strength, we find that a distinct Wigner crystal state is always stable at low filling. The results show that the scale invariance is explicitly broken. The observed Wigner crystal state illustrates that in 1D even short range interactions have an increasing effect with *growing* inter-particle spacing. The observed crossover is related to the so-called spin-incoherent Luttinger liquid[11].

Density oscillations can be calculated exactly for the non-interacting model $U = 0$ in a finite chain with "open" boundary conditions $\psi_{\sigma,0} = \psi_{\sigma,L+1} = 0$. The summation over standing waves $\sin(n \frac{\pi}{L+1} x)$ results in the well-known $2k_F$ Friedel oscillations [8]

$$\begin{aligned} \langle n(x) \rangle &= \frac{4}{L+1} \sum_{n=1}^{N/2} \sin^2(n \frac{\pi}{L+1} x) \\ &= \frac{2k_F}{\pi} - \frac{\sin(2k_F x)}{(L+1) \sin(\frac{\pi}{L+1} x)}, \end{aligned} \quad (2)$$

where the Fermi wave-vector $k_F = \frac{N+1}{2} \frac{\pi}{L+1}$ is centered between the highest occupied and lowest unoccupied level in a system with N fermions with spin. Here x is measured in units of the lattice spacing.

Possible Wigner oscillations can only appear at finite repulsive interactions $U > 0$ when fermions with opposite spin avoid each other. In the extreme case considered by Wigner all fermions would be arranged at maximum distances L/N apart. In the 1D case, the system remains critical but modulations with wave-vector $2\pi N/L \sim 4k_F$ will become important as we shall see later.

The Friedel oscillations are also modified by the interactions[12]. This can be seen by using the Luttinger liquid formalism as the low energy effective theory

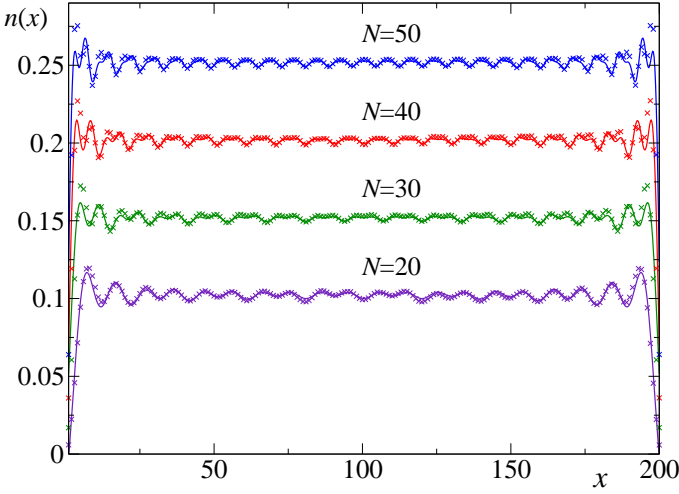


FIG. 1: Local density for $U = 4t$ and $L = 200$ for different filling showing the Friedel and Wigner crystal oscillations. The solid lines correspond to the theoretical prediction in Eq. (9).

[13] after linearization around k_F of the fermion fields $\psi_{\sigma,x} \approx e^{ik_F x} \psi_{R,\sigma} + e^{-ik_F x} \psi_{L,\sigma}$. In particular, using bosonization one can identify the Friedel oscillations as an expectation value of the operator

$$\begin{aligned} \mathcal{O}_{LR} &= \left(e^{i2k_F x} \psi_{L,\sigma}^\dagger(x) \psi_{R,\sigma}(x) + h.c. \right) \\ &\propto \sin(2k_F x + \sqrt{2\pi K_c} \varphi_c) \cos(\sqrt{2\pi} \varphi_s). \end{aligned} \quad (3)$$

Using the standard mode expansion of the spin field ϕ_s and the charge field ϕ_c , for finite systems[14, 15] the expectation value is determined to be

$$\langle \mathcal{O}_{LR} \rangle \propto \frac{\sin(2k_F x)}{\left[(L+1) \sin\left(\frac{\pi}{L+1} x\right) \right]^{(K_c+1)/2}}, \quad (4)$$

up to logarithmic corrections. The interactions change the decay rate of the Friedel oscillations compared to Eq. (2), which appear to be *enhanced* for repulsive interactions $K_c < 1$. However, as we will see, the yet undetermined amplitude also strongly depends on interactions and filling fraction.

The derivation of the Wigner oscillations from bosonization is more subtle. They arise from interactions because of the Umklapp term in the Hamiltonian density

$$\begin{aligned} \mathcal{O}_U &= g_3 \left(e^{i4k_F x} \psi_{R,\uparrow}^\dagger \psi_{L,\uparrow} \psi_{R,\downarrow}^\dagger \psi_{L,\downarrow} + h.c. \right) \\ &\propto \cos\left(4k_F x + \sqrt{8\pi K_c} \varphi_c\right), \end{aligned} \quad (5)$$

where $g_3 \propto U$. In first order perturbation theory this operator induces a density expectation value $\langle n \rangle_U = \langle n \rangle - \langle n \rangle_0$ relative to the unperturbed case

$$\langle n(x) \rangle_U \propto \int_0^L dy \sum_\alpha \frac{\langle 0 | \mathcal{O}_U(y) | \alpha \rangle \langle \alpha | \partial \varphi_c(x) | 0 \rangle}{E_\alpha - E_0} \quad (6)$$

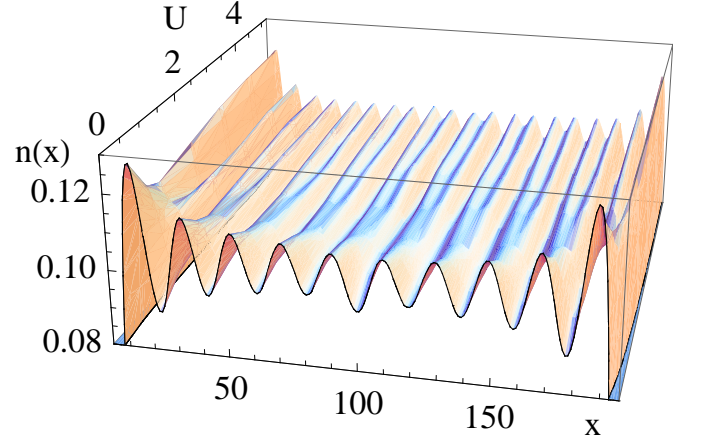


FIG. 2: Local density for $N = 20$ and $L = 200$ showing the crossover from $2k_F$ to $4k_F$ oscillations with increasing interaction strength U .

where $|\alpha\rangle$ are all excited states. By using the known mode expansion[15] it is possible to calculate the expectation values for all bosonic excitations $|\alpha\rangle$ with the result

$$\langle n(x) \rangle_U \propto \frac{g_3 K_c}{v_c} \int_0^L \frac{\sin(4k_F y) g(x, y)}{\left[(L+1) \sin\left(\frac{\pi}{L+1} y\right) \right]^{2K_c}} dy, \quad (7)$$

where $g(x, y) = \sum_{m=1}^L \frac{1}{m} \sin\left(\frac{\pi m}{L+1} y\right) \cos\left(\frac{\pi m}{L+1} x\right) \approx \frac{\pi}{2} \theta(y - x)$. Using $\int_0^\infty \sin(4k_F y) y^{-2K_c} dy \approx \cos 4k_F x / 4k_F x^{2K_c} + \mathcal{O}(x^{-2K_c-1})$ the integral can be approximated as[17]

$$\langle n(x) \rangle_U \propto \frac{g_3 K_c}{v_c k_F} \frac{\sin(4k_F - \frac{\pi}{L+1})x}{\left[(L+1) \sin\left(\frac{\pi}{L+1} x\right) \right]^{2K_c}}. \quad (8)$$

The decay rate for the $4k_F$ oscillations is faster than for the Friedel oscillations in Eq. (4) since $K_c \geq 0.5$ for the Hubbard model. The linear dependence on $g_3/k_F \propto UL/N$ is only accurate to lowest order in perturbation theory, but the typical oscillatory behavior and powerlaw will describe the behavior for any U and filling N/L . Alternatively, the *ad-hoc* inclusion of \mathcal{O}_U directly in the operator expression for the density is also a valid approach[6]. The explicit derivation from perturbation theory above now provides additional information by indicating an increase of the amplitude with g_3/k_F , i.e. with larger interactions and smaller filling. However, the exact amplitude cannot be derived from bosonization, so that numerical calculations have to be used.

We have implemented a DMRG algorithm [16] for the model in Eq. (1) in order to calculate the local density in finite systems with a given fermion number N . Typical densities at various fillings are shown in Fig. 1 for

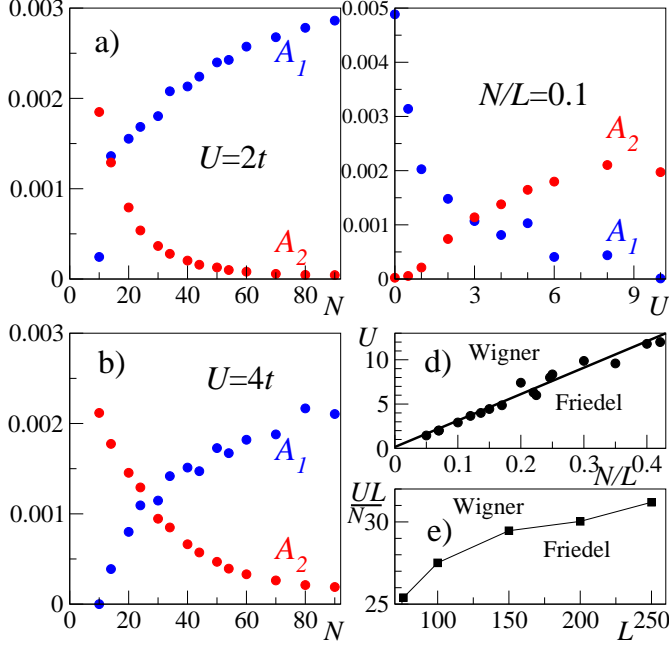


FIG. 3: Crossover of the amplitudes in Eq. (9) (error $\lesssim 10\%$) for $L = 200$ from the DMRG data as a function of filling and interaction. d) Crossover points ($A_1 = A_2$) in the U - N/L -plane showing the scaling with $UL/N \approx 30$ for $L = 200$. The solid line separates the Wigner and Friedel regions. e) Approximate crossover points UL/N as a function of length.

$U = 4t$ and $L = 200$, which clearly exhibit the predicted oscillations. Figure 2 shows how the local density at a given filling of $N/L = 0.1$ emerges from the slower Friedel oscillations to a Wigner crystal pattern as U increases.

An accurate data analysis is now possible in terms of our analytic predictions from Eqs. (4) and (8)

$$n(x) = n_0 - A_1 \frac{\sin(2k_F x)}{\left[\sin\left(\frac{\pi}{L+1}x\right)\right]^{\frac{K_c+1}{2}}} - A_2 \frac{\sin\left(4k_F - \frac{\pi}{L+1}\right)x}{\left[\sin\left(\frac{\pi}{L+1}x\right)\right]^{2K_c}}. \quad (9)$$

For arbitrary interactions $U > 0$ and filling N/L the Luttinger parameter $0.5 \leq K_c \leq 1$ can be calculated exactly[5, 6, 10], so that there are only two adjustable fitting parameters for the amplitudes in the middle of the chain A_1 and A_2 . For the non-interacting case in Eq. (2) we have $A_1 = \frac{1}{L+1}$ and $A_2 = 0$, which we can use as a test of the numerical accuracy. The uniform density n_0 is fixed by the requirement that $\int n(x)dx = N$, so that it is not an independent fitting parameter. (e.g. $n_0 = \frac{N}{L+1}$ for $U = 0$).

Figure 1 shows the quality of typical fits to the DMRG data. The oscillations in the middle of the chain are very well represented by the analytical expression (9), while there are small deviations near the edges. Deviations from Luttinger liquid theory near boundaries have also

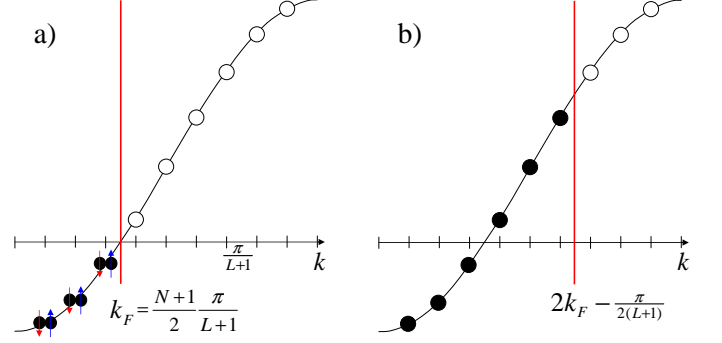


FIG. 4: Schematic occupied states for a) the nearly free case and b) for strong interactions ("Wigner crystal state").

been observed before in the context of the local density of states[18]. In order to determine the asymptotic amplitudes A_1 and A_2 as accurately as possible we have therefore excluded the first few sites near the ends in the fits. The fits are sensitive enough to even confirm the exact values of the wave-vectors $2k_F$ and $4k_F - \frac{\pi}{L+1}$, since small deviations of order $\frac{\pi}{L+1}$ already would make the quality of the fits considerably worse.

The results for the Friedel amplitude A_1 and the Wigner amplitude A_2 are shown in Fig. 3 for $L = 200$. The amplitudes show a clear crossover from Friedel oscillations to Wigner crystal waves at low filling. Interestingly, the Friedel oscillations are suppressed exactly when the Wigner crystal waves are strong and vice versa. Therefore, it is possible to identify two distinct "regions" of Wigner crystal and Friedel behavior. There is no true phase transition, but we observe distinctly different physical behavior in the two regions.

From the Luttinger liquid theory it is not *a priori* obvious why Friedel and Wigner oscillations cannot be strong simultaneously, but this competition can be understood in the momentum space picture. The Friedel oscillations in Eq. (2) are caused by the sum of standing waves in the two spin channels up to k_F as indicated in Fig. 4-a. The Wigner oscillations can be explained by an analogous picture, if it is assumed that fermions of opposite spin are not allowed to occupy the same orbital as shown in Fig. 4-b. The density of the "Wigner crystal state" is again given by a sum as in Eq. (2) where the index now runs over only one channel up to twice the wave-vector $2k_F$. Therefore, in Eq. (9) we have exactly $K_c = \frac{1}{2}$, $A_1 = 0$, and $A_2 = \frac{1}{2(L+1)}$, which is the maximally possible amplitude for Wigner oscillations. It is not possible to simultaneously have a Friedel and Wigner crystal state, leading to a natural competition between $2k_F$ and $4k_F$ oscillations in agreement with Fig. 3.

In our case, the Wigner crystal state in Fig. 4-b still has an equal number of spin up and down fermions. This is in contrast to charge density waves in ultracold gases

and Wigner crystals in higher dimensions, which typically tend to be spin polarized. In fact, it appears that the Wigner crystal state in Fig. 4-b can be realized for any magnetization, so that the correlations in the spin sector must be irrelevant. A small amplitude of spin-boson correlations also explains that the expectation of the Friedel operator in Eq. (4) is strongly suppressed in that regime. Hence, the Wigner crystal state in 1D signals the onset of spin-incoherent Luttinger liquid behavior with a nearly degenerate spin sector and a truly different physical behavior[11].

The results in Fig. 3 now indicate when the crossover $A_1 \approx A_2$ towards the spin-incoherent Wigner crystal state occurs. We observe scaling behavior in the limit of small filling in terms of the variable UL/N as shown in Fig. 3-d for $L = 200$, where the crossover occurs along a line with $UL/Nt \approx 30$. This means that a larger average particle distance L/N is equivalent to an increase of U . At first sight it appears rather counter-intuitive that the on-site interaction U should show a stronger effect as the average inter-particle distance L/N is increased. This behavior is special to one dimension since the total kinetic energy scales with $(N/L)^3$ at low filling, which becomes always smaller than the total interaction energy, which scales with $(N/L)^2$ as $N/L \rightarrow 0$.

From the Bethe ansatz we find that the Luttinger parameter for the Hubbard model also follows a scaling relation at low filling

$$K_c \approx 0.5 + \left(\frac{Nt}{UL}\right) 4 \ln 2 + \mathcal{O}\left(\frac{N^2}{L^2}, \frac{t^2}{U^2}\right). \quad (10)$$

However, the length dependence of the crossover points UL/N in Fig. 3-e violates the scaling behavior. For a given density N/L and interaction strength U all parameters in the Luttinger liquid theory (v_c, v_s, K_c) are fixed. Nonetheless, it is still possible to observe a crossover from Wigner to Friedel oscillations as a function of length (moving horizontally in Fig. 3-e). It is quite surprising that a critical model can cross over to different physical behavior as a function of length only, when all relevant parameters are fixed. This remarkable violation of scale invariance is not due to higher order operators, but comes from the competition between vastly different velocities in the spin and the charge sector. Note, that the spin-incoherent Luttinger liquid can be defined even at $T = 0$ as the *length-dependent* region when the ultraviolet spin cutoff v_s/a becomes smaller than the infrared charge cutoff v_c/L . In our analysis the curve in Fig. 3-e only signals the first onset of Wigner crystal behavior, so that we cannot predict the full analytic behavior from simple arguments. In general, it appears that the competition of spin and charge energy scales is a common behavior in Luttinger liquid physics. Therefore, the crossover between the different density oscillations discussed above is a generic signature of spin-charge separation in one dimension.

From the experimental side, Luttinger liquid behavior has so far only been seen in very special cases, such as carbon nanotubes [19, 20] or cleaved edge overgrowth wires[21]. There is some hope now that Luttinger liquid physics can also be realized with ultra-cold fermionic atoms in nearly ideal geometries formed by optical traps[22], which would have the advantage that the density distribution discussed here could in principle be detected directly using high resolution cameras, electron beams[23], or noise interference[24]. Fermionic gases can already be cooled down to less than 1/10 of the Fermi energy. The finite temperature will lead to a faster decay of the oscillations from the edges that can be accounted for in the theory[15]. In fact it would be interesting to study the system in a regime where all spin excitations are smaller than the temperature. This would be a perfect realization of the spin incoherent Luttinger liquid, leading to a complete vanishing of the Friedel oscillations while the Wigner oscillations remain. Hard edges can also be implemented by focused laser beams or trapped impurity atoms. Quantitative details of these issues will have to be discussed in future works.

In summary, we have systematically analyzed the local density distribution as a function of filling, interaction strength U , and system size in finite Hubbard chains. A combination of bosonization and DMRG calculations allows a detailed description of the density oscillations in terms of the quantitative formula (9). For small interactions and large fillings $2k_F$ Friedel oscillations A_1 dominate, while the Wigner crystal amplitude A_2 remains small. However, for smaller filling or increasing interactions the overall amplitude A_1 of the Friedel oscillations is strongly reduced while A_2 grows. This signals the crossover to a different physical region, which is described by a Wigner crystal state with no double occupancy of spin up and down fermions. The density oscillations we have described here are the most accessible feature to study the crossover towards the spin-incoherent Luttinger liquid in detail, e.g. using ultra cold fermionic gases in 1D optical traps.

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